

Peak Separation

NETZSCH Separation of Peaks is a program for evaluation of different types of data. With it, the experimental data are fitted as an additive superposition of peaks. This program allows the separation of overlapped peaks, using the profiles from the following peak types: Gaussian, Cauchy, Pseudo-Voigt (additive mixture of Gaussian and Cauchy), Fraser-Suzuki (asymmetric Gaussian), modified Laplace (double-sided rounded) and Pearson.

Application fields:

- thermal analysis (Differential Scanning Calorimetry and Thermogravimetric Analysis),
- UV/VIS spectroscopy,
- NIR and IR spectroscopy,
- NMR spectroscopy,
- X-ray small-angle scattering of polymers (for profile analysis with a Pseudo-Voigt profile, the Gauss component indicates the degree of crystallinity).

Data for evaluation can be presented in ASCII file with at least two columns. X-Column for the thermal analytical measurements is usually time or temperature. Y-Column can be presented as the signal of differential type like curves of DSC or DTA containing peaks or as the signal of the integral type like TG curve.

The software has the possibility to present the measured curve as the sum of several peaks. The number of peaks can be set by user or found automatically by the software.

Each single peak is characterized by three or four parameters:

- position,
- amplitude,
- half width,
- asymmetry (for Fraser-Suzuki profile and Laplace),
- slimness (for Pearson profile only).

The unknown parameters for each peak can be found by the software from the fitting of resulting curve with the measured curve. The model is fit to the experimental data by means of a hybrid GAUSS-NEWTON procedure, where a Marquardt method is combined with a step length optimization. If the customer has additional information about peaks, then this information can be used in the software as the limitations for parameters. It can be used for example for the situation where all peaks must be positive, or some of them must have no asymmetry, or if resulting signal contain peak with known parameters.

Stages of analysis

- I. **Data Loading and determination the range for analysis**
- II. **Baseline Correction** of the measured data. The baseline is corrected using Chebyshev's polynomial.
- III. **Separation of peaks with determination of peak parameters.** Separation can be done manually or automatically. Two equally remarkable features of the algorithm are speed and stability
 - i. **Manual Evaluation**
 - Set number of peaks
 - Set approximate position for each peak
 - Set type for each peak: : Gaussian, Cauchy, Pseudo-Voigt, Fraser-Suzuki or Pearson
 - Optimize peak parameters manually to get approximate values
 - Start optimization procedure to get exact values of parameters for each peak
 - ii. **Automatic evaluation**
 - Set number of peaks (if known) or set 'auto search' to find it automatically. The maximal number of peaks is 20.
 - Start optimization procedure to get exact values of parameters for all peaks

Example1: DSC melting peak of polypropylene fiber, first heating.

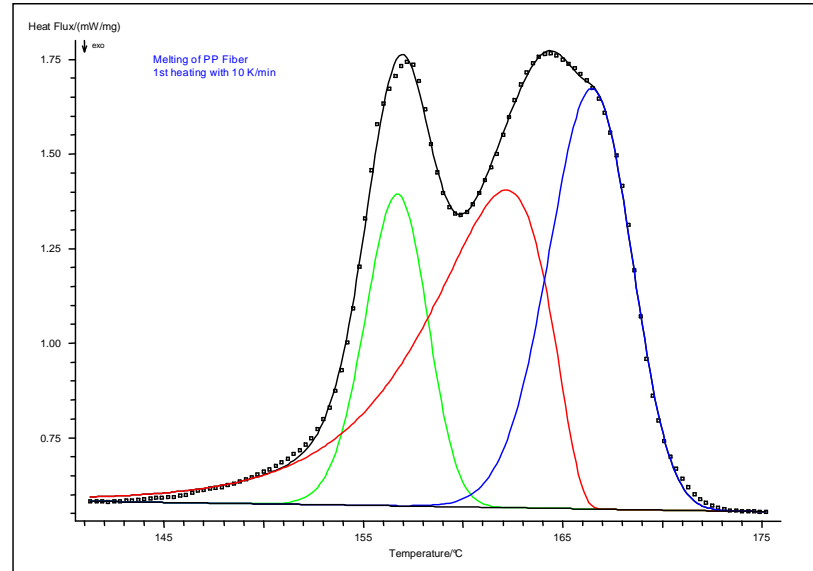
NETZSCH Peak Separation

Project: Melting of PP Fiber
 Instrument: NETZSCH DSC-DOS (Heat Flux)
 Identity: #PPFASER2 02-06-92 14:18
 ASCII File: PPFASER2.TXT
 Heating rate/(K/min): 10.000
 Min. X-Value: 141.3000
 Max. X-Value: 175.2000
 Date/Time: 20.07.2006 at 11:21

PEAK AREA, ONSET AND ENDSET

#	Shape	Position/°C	Area/(J/g)	PartArea%	Error/%	Onset/°C	Endset/°C
1	FRASER	156.7117	19.3387	20.092	2.475	153.459	159.698
2	FRASER	162.1845	42.2567	43.904	14.439	153.718	165.969
3	FRASER	166.4699	34.6534	36.004	9.317	162.092	170.378

NETZSCH Peak Separation Project: Melting of PP Fiber



The DSC melting peak of a polypropylene fiber clearly displays two maxima in the first heating. The second of them belongs to the double peak. All peaks are fitted by means of FRASER-SUZUKI peak type.

Example2: DSC melting peak of palm oil.

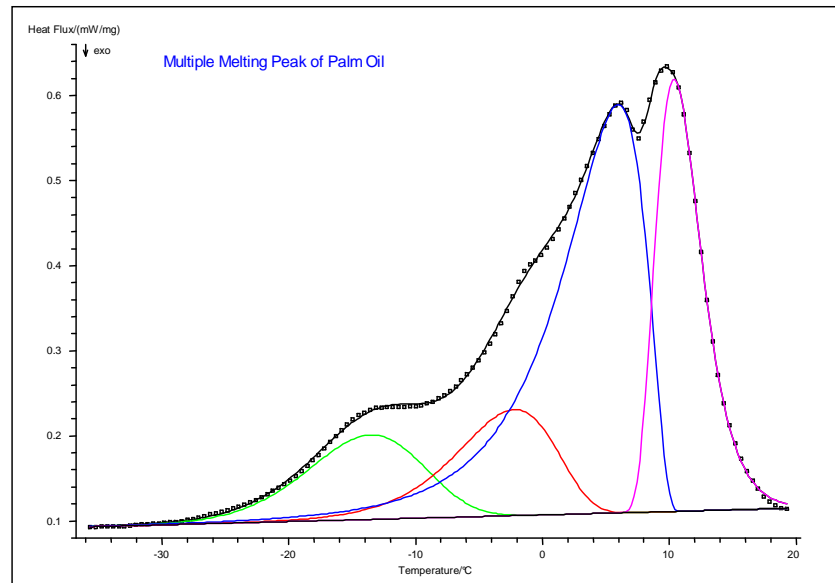
NETZSCH Peak Separation

Project: Palm Oil
 Instrument: NETZSCH DSC-DOS (Heat Flux)
 Identity: #1859111 05-12-91 11:07
 ASCII File: PALM-OIL.TXT
 Heating rate/(K/min): 10.000
 Min. X-Value: -35.6500
 Max. X-Value: 19.2500
 Date/Time: 20.07.2006 at 11:30

PEAK AREA, ONSET AND ENDSET

#	Shape	Position/°C	Area/(J/g)	PartArea%	Error/%	Onset/°C	Endset/°C
1	FRASER	-13.5425	6.8559	12.404	12.365	-23.707	-5.428
2	FRASER	-2.2135	7.5586	13.675	21.886	-11.743	3.999
3	FRASER	5.9791	26.5431	48.023	6.222	-3.353	9.895
4	FRASER	10.3741	14.3140	25.897	1.443	7.575	14.852

NETZSCH Peak Separation Project: Palm Oil



The DSC melting peak of a palm oil displays four peaks corresponding to melting of different components.

For the complex curves the user can set only number of peaks. Then these peaks will be found automatically

Results of the evaluation:

- the optimal parameters for each peak and their standard errors,
- statistical characteristic values such as the correlation coefficient and the average fit error,
- graphic representation of the curve fit including the separated single peaks,
- calculation of the areas of the each single peaks and their percentage of the total peak.

For analysis according to good laboratory practice (GLP) all parameter of analysis are shown in the heading of result list.

Additional information can be found on www.therm-soft.com